2-Methylhexane
591-76-4 | DTXSID5052256

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 5.54 days

Global applicability domain: Inside

Local applicability domain index: 8.50e-01

Confidence level: 7.20e-01

Nearest Neighbors from the Training Set

Image not found	Image not found	Image not found
2-Methylhexane	3-Methylhexane	4-Methyloctane
Measured: 12.5	**Measured:** 157	**Measured:** 40.7
Predicted: 5.54	**Predicted:** 6.83	**Predicted:** 3.58